LA-UR-00-5312

Approved for public release; distribution is unlimited.

Title: A NEW NUCLEAR STRUCTURE LIBRARY FOR MCNPX AND LAHET3

Author(s): R E Prael

Submitted to: Imbedded topical meeting Accelerator Applications 2000, American Nuclear Society meeting November 12-16, 2000

Los Alamos
NATIONAL LABORATORY

A NEW NUCLEAR STRUCTURE LIBRARY FOR MCNPX™ AND LAHET3™
(LA-UR-00-5312)

R. E. Prael
Los Alamos National Laboratory
P. O. Box 1663
Los Alamos, NM 87545
(505) 667-7283

ABSTRACT

A new nuclear structure data library will be released for use with MCNPX. The library is intended to enable estimation of metastable state production, correlated with the contents of the CINDER'90 data library. When used with MCNPX, the residual nucleus production estimates may be provided as input to the CINDER'90 code.

I. INTRODUCTION

One of the objectives of the code development effort supported by the Accelerator Production of Tritium program is to estimate the production of metastable isotopes with an MCNPX[1] particle transport calculation and to provide the results as input for a subsequent CINDER'90[2] calculation to follow time-dependent decay. The necessary predictive capability is a function of the nuclear structure data library used in the gamma emission process following all particle emission processes. The procedures to be followed in constructing such a data library have been described previously.[3] Since all the features necessary to utilize such a library are now available in MCNPX, the current version (designated SPEC1) is being made available for use with MCNPX.

II. CHARACTERISTICS OF THE SPEC1 NUCLEAR STRUCTURE LIBRARY

In general, for de-excitation of a nucleus after nucleon and ion emission is terminated, the emission process follows branching ratios from the library where known, including internal transitions, terminating at delayed particle emission (β, α or nucleon) or electron capture. The procedure uses spin and parity information in the library to calculate branching in the gamma cascade when branching ratios are not available. To achieve the objective of estimating metastable state production, the SPEC1 library is constructed to terminate the emission process at nuclear levels with $t_{1/2} \geq 1$ ms. The latter criterion is a major departure from the original procedure used with LAHET and MCNPX, where all gamma-emitting states were allowed to decay with appropriate sampling of the emission time.

The BUDAPEST_LEVELS.DAT file, compiled by G. Molnar *et al.*, was obtained from the RIPL project library[4] to provide the basis for the new data library. The procedure described above was used to prevent decay from states with $t_{1/2} \geq 1$ ms. A preliminary comparison of the initial library (PHTLIB/RIPL) with the contents of the CINDER'90 library indicated that data for many isotopes were completely absent in the BUDAPEST_LEVELS.DAT file. To improve the match with the CINDER'90 library, data for 45 isotopes were copied from the original PHTLIB file generated from the CRDL[5] structure data. Conflicts and uncertainties in identifying the metastable states as defined in the new library with levels in the CINDER'90 library were resolved by reference to the tabulations of Firestone and Shirley.[6] The latter was also used to add information about low-lying levels not otherwise present. The final version containing these elements has been designated as PHTLIB/SPEC1.

Information in the SPEC1 library allows the identification of the estimated final state population with specific levels in the CINDER'90 library. The characteristics of the library are:

- 623 metastable states defined according to the criteria defined above;
- 567 states identified with a first level for an isotope in the CINDER'90 library;
- 56 states identified with a second level for an isotope in the CINDER'90 library;
- 67 states from the above not presently in the CINDER'90 library.

Future development will depend on the creation of a *new* version of the CINDER'90 library. In that case, the

remaining discrepancies may be reduced and a new version ("SPEC2") released.

Editing isotopic production information from an MCNPX or LAHET3 calculation provides the fraction of metastable state production; the detailed state estimates may be written as a file intended as input to CINDER'90. Until such time as the missing data are added to the CINDER'90 library, population of the 67 unmatched states will be identified with the isotopic ground state when results are passed from an MCNPX or LAHET3 calculation as an input source for CINDER'90.

III. COMPUTATIONAL EXAMPLES

The calculations shown in table 1 were made with LAHET3 and are estimates of the fraction of isotopic production appearing in the metastable state for an 800 MeV proton beam incident on a massive natural iron beam stop. The results shown for the calculation with the new SPEC1 library represent 484013 proton histories; the calculations made with the original nuclear structure library represent 100000 proton histories. Performing the calculation with the SPEC1 library provides an estimate for the production of seven states not identified in the calculation using the original data library. In this example, all the states shown for the SPEC1 calculation are identified with the *first* metastable level for that isotope in the CINDER'90 library. Note that the excitation energies and half-lives shown in the table are the values included in the SPEC1 data.

A second comparison was made for the case of 256 MeV protons incident on a stopping length target of ^{238}U. Although the full comparison is too lengthy to reproduce in this paper, the results from a 100,000 history calculation indicate that

1. with the SPEC1 library, estimates for the production of 360 metastable states were obtained;
2. with the original library (allowing gamma emission from metastable states), only 147 states were identified;
3. with the original library, modified as above to block gamma emission from metastable states, production estimates for 292 metastable states were obtained.

The difference between (1) and (3) reflects the improved physical data present in the new SPEC1 library; the difference between (2) and (3) represents the change in the method for using the data present.

IV. CONCLUSIONS

As noted above, the use of the SPEC1 library provides an extended predictive capability for MCNPX or LAHET calculations. One may also note in table 1 that the use of contemporary data provides a significantly different prediction for the production rates of some metastable states, notably ^{52}Mn. The SPEC1 library is available for use with the most recent release of MCNPX and with LAHET2.8,[7] and, with some small code modifications, could be used with LAHET2.7. In addition, the SPEC1 library may be of interest for use with other codes that have adopted the gamma de-excitation methods from the LAHET Code System.

REFERENCES

1. H. G. Hughes *et al*., "The MCNP/LCS Merger Project", *Topical Meeting on Nuclear Applications of Accelerator Technology*, Albuquerque, NM, November 1997, American Nuclear Society, La Grange Park, Illinois, p. 213 (1997).

2. W. B. Wilson *et al*., "CINDER'90 Code for Transmutation Calculations", *Proceedings of the Inter-national Conference on Nuclear Data for Science and Technology*, Trieste, 19-24 May 1997, Italian Physical Society, Bologna, p. 1454 (1997).

3. R. E. Prael and W. B. Wilson, "Nuclear Structure Libraries for LAHET™ and MCNPX™," *Proceedings of the 4th Work-shop on Simulating Accelerator Radiation Environments*, Sept. 13-16, 1998, Knoxville, Tennessee, Oak Ridge National Laboratory, p. 183 (1998)

4. M. B. Chadwick *et al*., *Reference Input Parameter Library: Handbook for Calculations of Nuclear Reaction Data*, IAEA-TECDOC-Draft, IAEA, Vienna (March 1998).

5. R. J. Howerton, *ENSL and CDRL: Evaluated Nuclear Structure Libraries*, UCRL-50400, Vol. 23, Lawrence Livermore National Laboratory (February 1981).

6. R. B. Firestone and V. S. Shirley, *Table of Isotopes: Eighth Edition*, John Wiley, New York (1996).

7. R. E. Prael and D. G. Madland, *The LAHET Code System with LAHET2.8*, report LA-UR-00-2140, Los Alamos National Laboratory (January 2000).

Z	A	E(level) (MeV)	$t_{1/2}$ (sec)	Fraction (SPEC1)	Relative Error	Fraction (original)	Relative Error
11	24	0.4722	2.020D-02	7.20D-01	0.046	9.28D-01	0.071
13	26	0.2283	6.345D+00	6.16D-01	0.024	6.08D-01	0.053
17	34	0.1463	1.920D+03	3.65D-01	0.041	1.89D-01	0.104
17	38	0.6713	7.150D-01	1.18D-01	0.042	absent	
19	38	0.1304	9.239D-01	5.46D-01	0.034	5.00D-01	0.073
21	42	0.6162	6.170D+01	3.47D-01	0.054	1.08D-01	0.139
21	44	0.2711	2.110D+05	6.87D-02	0.008	absent	
21	45	0.0124	3.180D-01	6.56D-01	0.004	absent	
21	46	0.1425	1.875D+01	3.59D-01	0.008	absent	
21	50	0.2568	3.500D-01	8.46D-01	0.109	absent	
23	46	0.8015	1.020D-03	4.74D-01	0.035	absent	
25	50	0.2290	1.050D+02	3.42D-01	0.040	3.62D-01	0.083
25	52	0.3777	1.266D+03	6.92D-01	0.002	1.33D-01	0.008
26	53	3.0404	1.548D+02	3.68D-03	0.009	absent	
27	54	0.1990	8.880D+01	2.06D-01	0.035	1.66D-01	0.074

Table 1: Comparison of calculated metastable state production as a fraction of isotopic production for 800 MeV protons on a natural Fe beam stop.